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DEFORMATION, CONSTITUTIVE BEHAVIOR AND DAMAGE OF ADVANCED
STRUCTURAL MATERIALS UNDER MULTIAXIAL LOADING

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TABLE OF CONTENTS

I. PROGRAM OVERVIEW	1
II. INTRODUCTION	1
A. DEFORMATION CHARACTERISTICS OF SINGLE CRYSTAL NiAl	1
1. Effect of Orientation	1
2. Effect of Stress States	1
B. DEFORMATION CHARACTERISTICS OF POLYCRYSTALLINE NiAl	2
1. Below BDTT	2
2. Above BDTT	3
3. Effect of Stress States	3
III. PROGRESS DURING PERIOD JUNE 1,1992-JUNE 30,1993	4
A. POLYCRYSTALLINE NiAl	4
1. Multiaxial Testing	4
2. Compression Testing	4
3. Results and Discussion	4
B. SINGLE CRYSTAL NiAl	5
1. Theoretical Considerations	5
IV. WORK PLANNED DURING NEXT PERIOD	6
A. FEA	7
B. MECHANICAL TESTING	7
C. SEM	8
D. TEM	8
V. INTERACTIONS WITH OTHER INVESTIGATORS	8
VI. PERSONNEL	8
VII. REFERENCES	10

I PROGRAM OVERVIEW

In the grant period just completed (06/01/92-09/30/93), the metallurgical variables identified in the previous period have been addressed. Room temperature multiaxial testing of polycrystalline NiAl has been completed and high temperature experiments are being planned. In addition, compression testing of polycrystalline NiAl at room temperature has also been done. These experiments were included in the program to further investigate the results of the multiaxial experiments. The prime objective of these experiments is to differentiate damage and plasticity observed in this material under compression. Finite element analysis based on micromechanics will be done to study the stress distribution at the grain boundaries. Together, these experiments will form the basis for development of a constitutive model which takes into consideration crystal plasticity and damage.

II INTRODUCTION

A. Deformation Characteristics of Single Crystal NiAl

1. Effect of Orientation

For "soft" orientation single crystals, $\langle 001 \rangle$ slip vector dominates and flow stress is relatively low (40-100MPa)[1]. For "hard" orientation single crystals, the $\langle 111 \rangle$ slip vector dominates and the flow stress is higher. However, in both cases, negligible room temperature ductility is observed due to low cleavage strength which causes failure prior to yielding.

2. Effect of Stress States

NiAl behaves differently in tension and compression. Ball and Smallman[2] reported extensive room temperature ductility for NiAl single crystals which had been widely misrepresented as tensile ductility. However, these results were observed for $\langle 110 \rangle$ single crystals tested in compression and are thus not representative of true ductility of the material as non- $\langle 110 \rangle$ oriented single crystals exhibit significantly different compressive ductilities. "Hard" orientations single crystals which deform by $\langle 111 \rangle$ slip have compressive ductilities no greater

than 16%[3,4]. Irrespective of orientation, NiAl single crystals exhibit negligible room temperature tensile ductility.

B. Deformation Characteristics of Polycrystalline NiAl

Besides stoichiometry and composition, temperature also affects the mechanical response of NiAl. Ductility increases significantly above the brittle-to-ductile transition temperature (BDTT) which is defined as the temperature at which 5% tensile ductility is observed[5]. Figure 1. shows the observed change in tensile ductility as a function of temperature for NiAl. Due to the significant ductility enhancement above the BDTT, the following discussion will initially focus on the low temperature "brittle" behavior, and then the high temperature "ductile" regime.

1. Below BDTT

It is generally agreed that the operative slip system in polycrystalline NiAl is $\langle 001 \rangle \{110\}$ which provides only three independent slip systems, thus failing to satisfy von Mises criteria for generalized plasticity. Compression tests on NiAl indicate that limited slip systems in NiAl lead to grain boundary cracking and subsequent failure[6]. In addition to a lack of five independent slip systems, brittleness in NiAl has also been attributed to weak grain boundaries. This was determined from studies conducted to investigate the effect of B additions on ductility and fracture of NiAl[7]. Stoichiometric NiAl failed intergranularly with limited tensile ductility. Auger analyses revealed that the grain boundaries were clean and free of impurities, implying that inherently weak grain boundaries contribute to brittle failure. Boron additions segregated to grain boundaries and suppressed intergranular fracture. However, these additions failed to increase room temperature ductility, due to solid-solution strengthening which significantly increased the yield strength and produced fracture prior to yielding.

2. Above BDTT

As shown in Figure 1, with increasing temperature, the ductility of NiAl increases at a characteristic temperature defined as the BDTT. It has been argued that either thermally activated deformation processes such as climb[5,8-10] or activation of additional slip systems[11] leads to the observed change in deformation behavior above BDTT. Groves and Kelly[12] initially demonstrated that a combination of climb and glide can result in five independent deformation modes which would then satisfy the von Mises criterion for generalized plasticity. Alternatively, observations of $a\langle 110 \rangle$ dislocations on $\{110\}$ planes in compressed bicrystals resulted in the speculation that activation of additional slip systems was responsible for the observed increased ductility above the BDTT. However, it is argued that if the change from brittle to ductile behavior was due to the activation of additional slip systems at some critical temperature, then the BDTT is should be strain rate independent. It is experimentally observed that the BDTT is strongly strain rate dependent with an increase of approximately 200K for three orders of magnitude increase in strain rate[5] which strongly favors thermally activated deformation mechanisms to be responsible for the increase in ductility above the BDTT. Furthermore, results of extrinsic grain boundary dislocation (EGBD) annealing study indicate activation of diffusional processes around the BDTT, during which grain boundary dislocations were observed to be mobile precisely at the BDTT[9].

3. Effect of Stress State.

NiAl, in single and polycrystalline forms, behaves differently when tested in compression and tension. NiAl exhibits limited room temperature ductility in tension but exhibits significant plastic deformation when tested in compression. It should be noted that when tested in compression damage starts to accumulate at low strain levels at grain boundaries[10]. It is argued that stress state determines the ease of crack propagation and thus ductility. Consequently, the effect of stress state on plastic deformation of polycrystalline NiAl will be investigated at room and elevated temperatures.

III. PROGRESS DURING PERIOD JUNE 1, 1992 - JUNE 30, 1993

A. Polycrystalline NiAl

1. Multiaxial Testing

Table 1 describes the experimental test matrix for multiaxial testing of polycrystalline NiAl. The tensile tests were carried out to establish baseline ductility. Following these tests, pure torsion and non-proportional compression-torsion tests were carried out. A significant difference in the room temperature fracture morphology was observed (Figure 3.) for these experiments. In case of tension and torsion tests the failure mode was predominantly transgranular cleavage whereas for the case of non-proportional loading (torsion with axial compression) the failure mode was predominantly intergranular.

2. Compression Testing

In view of the new and interesting observation regarding the loading path dependence of fracture mode, it was obvious that more experimental work is needed to explain the observed high ductility when the specimen is compressed while applying a torsional load. It is also important to determine whether the observed high inelastic strains are due to dislocation motion or microcracking. In order to accomplish this, compression tests were carried out to various strain levels to cause grain boundary cracking but preclude failure. Figure 2 shows the stress strain curve of an incremental compression test carried out to 4% total strain.

3. Results And Discussion

Figure 3 shows the fracture surfaces of tested specimens. Specimens tested under pure tension and pure torsion failed via cleavage whereas a specimen tested under non-proportional compression-torsion loading failed in a predominant intergranular fashion. It also exhibited maximum plasticity ($\epsilon_{eq}=0.65\%$).

In case of pure tension and pure torsion experiments, the cleavage strength was exceeded

before any macroscopic yielding. But it is believed that in non-proportional compression-torsion experiment, the compressive load inhibited propagation of cleavage cracks. However, it is not clear whether the observed compressive ductility is due to plastic deformation or due to microcracking. In order to investigate this, several room temperature compression tests including an incremental compression test were carried out to investigate the onset of grain boundary cracking and thus separate out the contribution of deformation and damage to the macroscopically observed plastic strain. Figure 2 shows the stress strain curve of the incremental test carried out upto 4% total strain. Strains higher than 4% could not be achieved due to buckling. However, no grain boundary cracks were observed in specimens tested. This indicates that the observed high inelastic strains could be due to dislocation motion. However, further TEM investigation is required to determine the dislocation activity in tested specimens. These experiments will be repeated using a different specimen geometry to prevent buckling which will then allow desired plastic strain levels to be achieved.

B. Single Crystal NiAl

1. Theoretical Considerations

Figure 4 shows the transverse cross-section of an NiAl single crystal tubular specimen with [001] axial orientation; the figure indicates the changes in crystallographic orientation with angular position within the specimen. For [001] oriented single crystal, the resolved shear stress (RSS) under tension on $\langle 001 \rangle \{110\}$ slip system is zero or near zero (dependent upon the exact crystallographic orientation). Under such conditions, NiAl single crystals have been observed to deform by $\langle 111 \rangle$ Burgers vector on $\{110\}$, $\{123\}$ and/or $\{112\}$ [13-17] planes with an average shear stress of approximately 500MPa [18]. When the same crystal is deformed under pure torsion, an appreciable RSS exists on the $\langle 001 \rangle \{110\}$ slip system. However, the magnitude of this stress will vary along the circumference of the specimen (figure 4), as the angle between the applied shear stress (which is always tangential to the radius of the specimen) and a given crystallographic orientation changes with rotational angular position. This geometric relationship

gives rise to the possibility that different slip systems can be activated along the circumference of the crystal (i.e. deformation would be in homogeneous).

Thus, uniaxial tension on the [001] crystal results in $\langle 111 \rangle$ slip, while pure torsion should promote deformation by dislocations with $\langle 001 \rangle$ Burgers vector on $\{110\}$ type planes. At present, simultaneous operation of $\langle 111 \rangle \{110\}$ and $\langle 001 \rangle \{110\}$ slip systems has not been observed under uniaxial loading conditions since the CRSS for $\langle 111 \rangle \{110\}$ slip is approximately 3-5 times higher than that for $\langle 001 \rangle \{110\}$ slip [11]. However, it is possible that under multiaxial loading a particular ratio of axial to shear stresses (designated λ) may be chosen such that the RSS on the $\langle 001 \rangle \{110\}$ and $\langle 111 \rangle \{110\}$ slip systems exceeds their corresponding CRSS, causing simultaneous activation. Figures 5 to 8 show the calculated maximum resolved shear stress on the $\langle 001 \rangle \{110\}$ and $\langle 111 \rangle \{110\}$ slip systems as a function of angle around the specimen circumference from the [100] direction. These figures show the maximum stress on a family of slip systems, where the troughs indicate a change in the active slip system. Figure 5 represents the case of pure tension with $\lambda = \infty$ and a $\langle 111 \rangle$ slip vector should operate. In contrast, figure 6 represents pure torsion where $\lambda = 0$. In this case the crystal would lose its "hard" orientation and thus be able to deform by a $\langle 001 \rangle$ Burgers vector. Figure 7 shows the RSS on the two slip systems for an applied $\lambda = 0.5$. In this case, the RSS on the $\langle 001 \rangle \{110\}$ slip system is considerably lower than for the case of pure shear. Finally, figure 8 shows the RSS for $\lambda = 0.2$ which yields a ratio of the RSS on the two slip systems which is the same as the shear yield ratios. This could cause simultaneous activation of the two slip systems (i.e. $\frac{CRSS_{\langle 001 \rangle}}{CRSS_{\langle 111 \rangle}} \equiv 0.20$)

Owing to difficulties in obtaining single crystal NiAl specimens, mechanical testing of single crystal NiAl specimens will not be addressed in this research period.

IV. WORK PLANNED DURING THE NEXT PERIOD

Results from the previous period indicate that the state of stress plays a profound role in the mechanism of cracking. A research course is proposed for the next period which consists of well directed experiments to address the influence of variables identified earlier. These experiments will

also address questions raised by the research conducted so far. Details are discussed below.

1. Finite Element Analysis (FEA): Clearly, intergranular cracking appear to play a strong role in ductility enhancement during non-proportional loading at room temperature. Stresses induced by misorientation at grain boundaries likely play a key role in this process. The modeling effort will attempt to demonstrate the role of stress-state dependent microcracking on inelastic strain accumulation at room temperature. Moreover, the transition to diffusional climb-controlled rate-dependent behavior above the BDTT will be addressed.

Assemblages of grains will be analyzed under elastic conditions to establish the energy associated with grain misorientation as a function of stress-state. The isostrain assumption will be made for an assemblage of grains. In addition, three-dimensional finite element analyses will be used to assess grain boundary stress distributions. Based on these results, microcracking model will be developed which is consistent with reducing elastic energy associated with misorientation. The model must also address the issues of stable intergranular crack growth and catastrophic cleavage failure. The model will be evaluated on the basis of further nonproportional loading tests with periodic unloading and damage evaluation.

2. Mechanical Testing: As discussed earlier, stress-state also affects high temperature behavior of NiAl. Thermally assisted deformation processes such as climb have been proposed as the mechanism for increased ductility above the BDTT. Elevated temperature experiments are planned to further validate the proposed mechanism. The process of climb can be either enhanced or retarded by maximizing or minimizing hydrostatic stresses. The state of hydrostatic stress can be controlled by the loading paths selected (Table 1 describes the various loading paths). In-phase tension-torsion loading will maximize the hydrostatic stress and in-phase compression -torsion loading will minimize the hydrostatic stress.

Additional testing will be carried out in which the loading paths are changed in order to alter crack growth mechanisms to validate the predictions and/or results of numerical analyses.

3. **SEM:** Predictions of finite element analysis regarding the dominant fracture mode will be investigated by studying the fracture surface morphologies of the failed specimens.

4. **TEM:** The plastic deformation is controlled by dislocation movement. TEM analysis will be done to investigate the various deformation mechanisms operating under different loading conditions at room and elevated temperatures. Such an investigation will give further insight into the role of different operating slip systems on the mechanism of cracking in this material.

V. INTERACTIONS WITH OTHER INVESTIGATORS

Close working relationships have been established with other institutions and industries. In particular the following interactions are taking place:

1. Dr S. D. Antolovich of Washington State University is serving on the dissertation committee and continues to provide advice on various aspects of the single and polycrystalline program.

2. Dr Randy Bowman, NASA Lewis Research Center, has supplied NiAl materials and has also provided advice as to experiments that would complement work at NASA. Dr Bowman received his Ph.D in 1988 and did his dissertation work on an AFOSR project.

3. Discussions are under way between Dr Antolovich and Ram Darolia of General Electric, Evendale, Ohio, to obtain single crystals for deformation studies.

VI. PERSONNEL

Dr D. L. McDowell, Director, MPRL and Professor, School of Mechanical Engineering, is the principal investigator and is responsible for the overall management of the project.

Dr Graham Webb completed his Ph. D in August 1991. He provided technical assistance as a post-doctoral research fellow from January 1993 to June 1993.

Mr Ritesh Shah is a Graduate Research Assistant who started his Ph.D program in January 1991. He is responsible for mechanical testing and for computer modeling of deformation processes. While working on various aspects of the project, Mr Shah presented his Ph.D proposal.

Mr Rick Brown is a Research Equipment Specialist in the Mechanical Properties Research Laboratory at Georgia Institute of Technology and is involved with experimental set-ups and assisting and training students.

In addition to the above personnel, clerical assistance has been provided by Ms. Susan Bowman. Administrative and financial assistance is provided by Ms. Pat Ledon and Ms. Robin Greene, all of the school of Materials Engineering.

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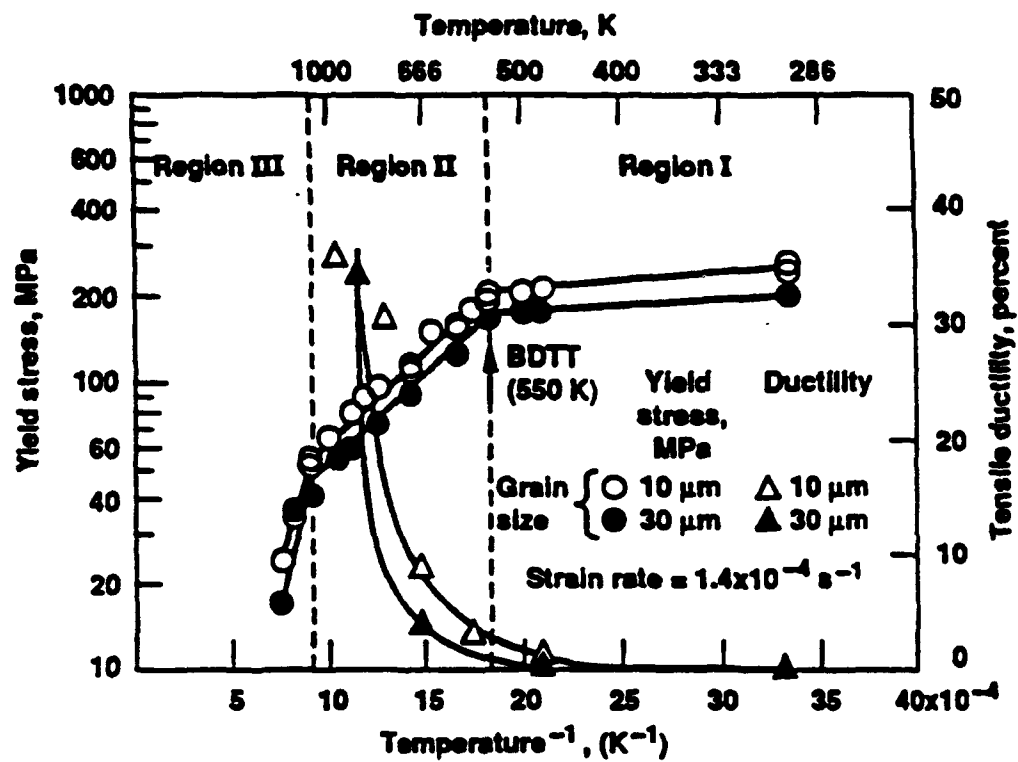


Figure 1. Brittle to ductile transition behavior of powder extruded NiAl[6]

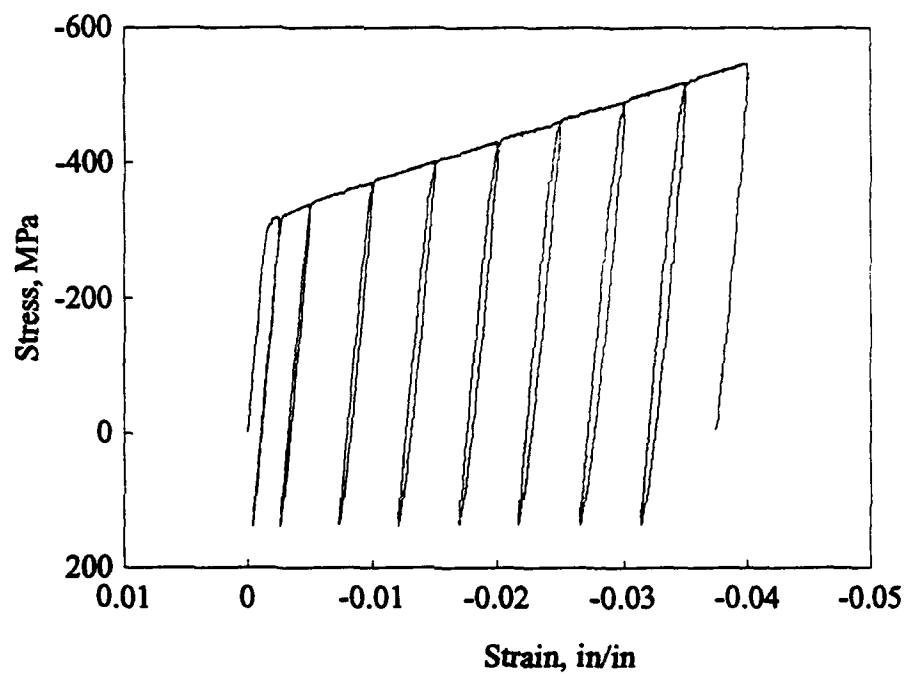
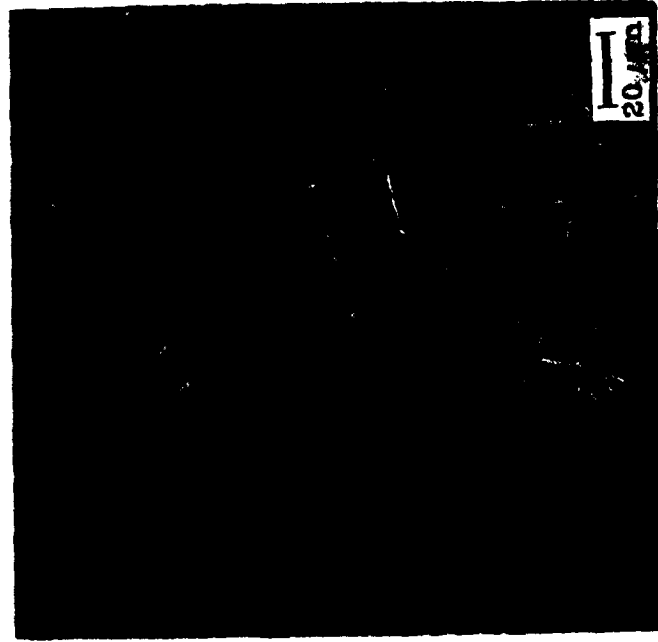


Figure 2. Stress-strain response of polycrystal NiAl subjected to incremental compressive strain at room temperature.



Pure Tension

$$\epsilon_f^{\text{tot}} = 0.26\%$$

$$\epsilon_{pl} = 0.17\%$$



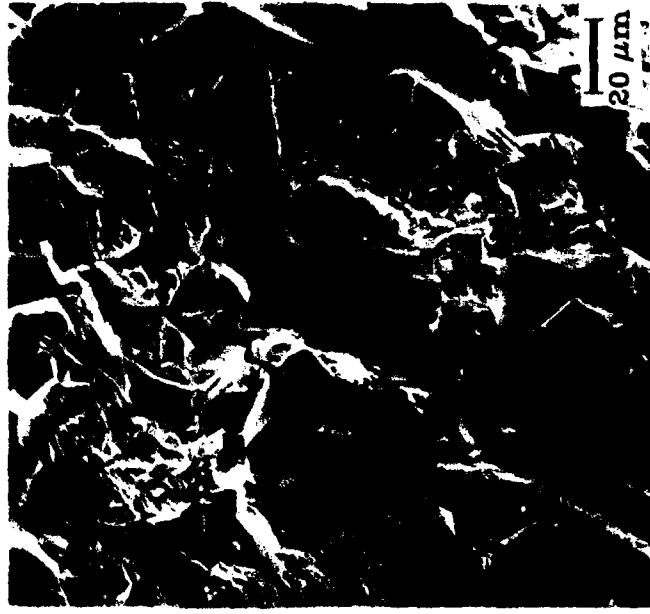
Pure Torsion

$$\gamma_f^{\text{tot}} = 0.6\%$$

$$\gamma_{pl} = 0.43\%$$

$$\epsilon_{eq}^{\text{tot}} = 0.35\%$$

$$\epsilon_{eq}^{pl} = 0.25\%$$



Torsion With Axial Compression

$$\gamma_f^{\text{tot}} = 1.3\%$$

$$\gamma_{pl} = 1.05\%$$

$$\epsilon_{eq}^{\text{tot}} = 0.75\%$$

$$\epsilon_{eq}^{pl} = 0.65\%$$

Figure 3: Fracture surfaces of failed specimens and corresponding strains.

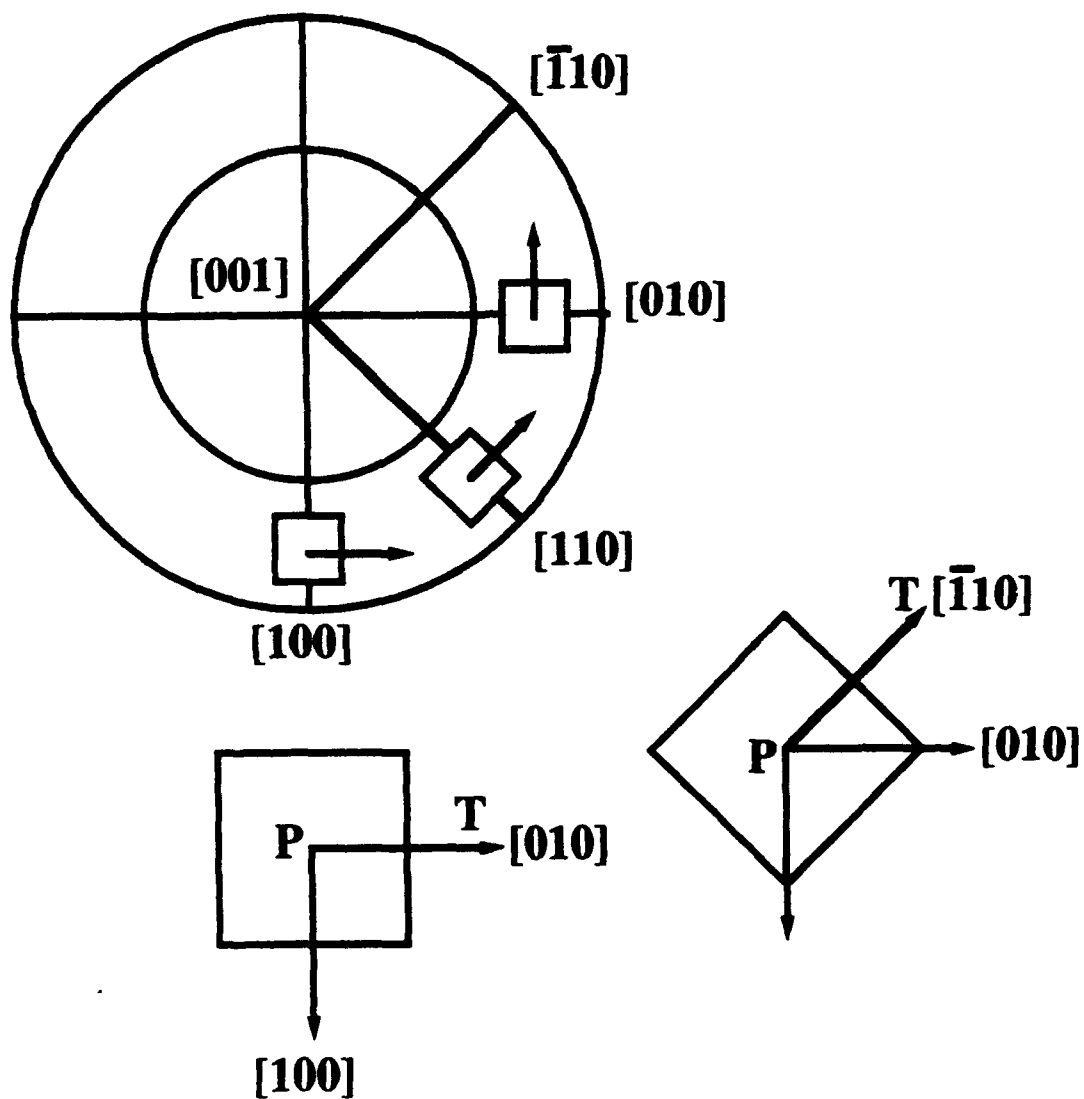


Figure 4. Transverse cross section of single crystal specimen indicating the changes in the crystallographic orientation with angular position and the relationship between applied load and crystallographic direction.

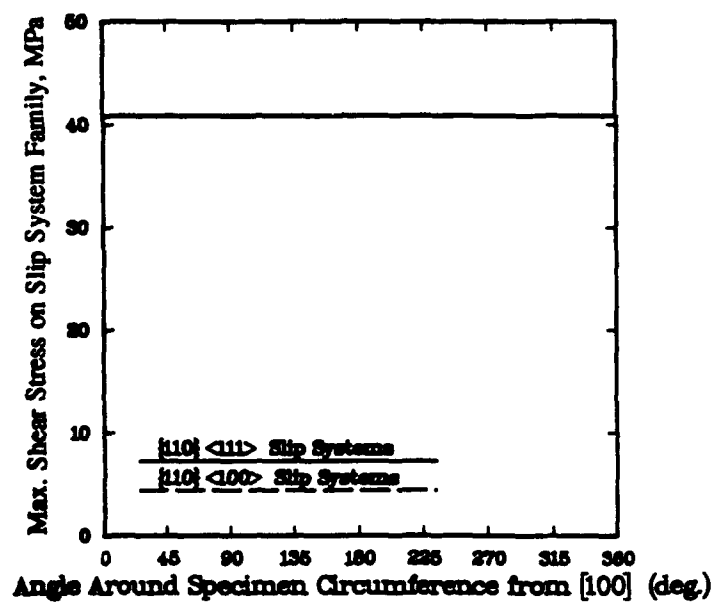


Figure 5. Maximum resolved shear stress on $\langle 111 \rangle \{110\}$ and $\langle 001 \rangle \{110\}$ families of slip systems, $\lambda = \infty$ (Pure Tension)

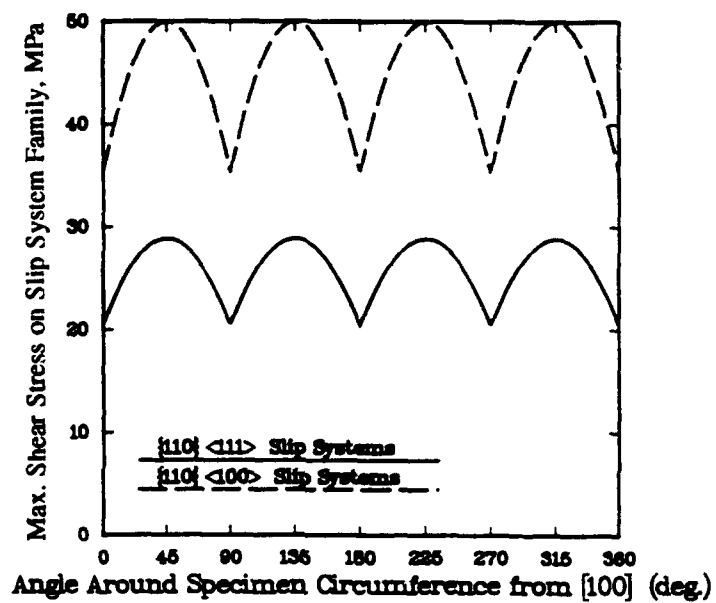


Figure 6. Maximum resolved shear stress on $\langle 111 \rangle \{110\}$ and $\langle 001 \rangle \{110\}$ families of slip systems, $\lambda=0$ (Pure Torsion). The troughs represent a change in the slip system.

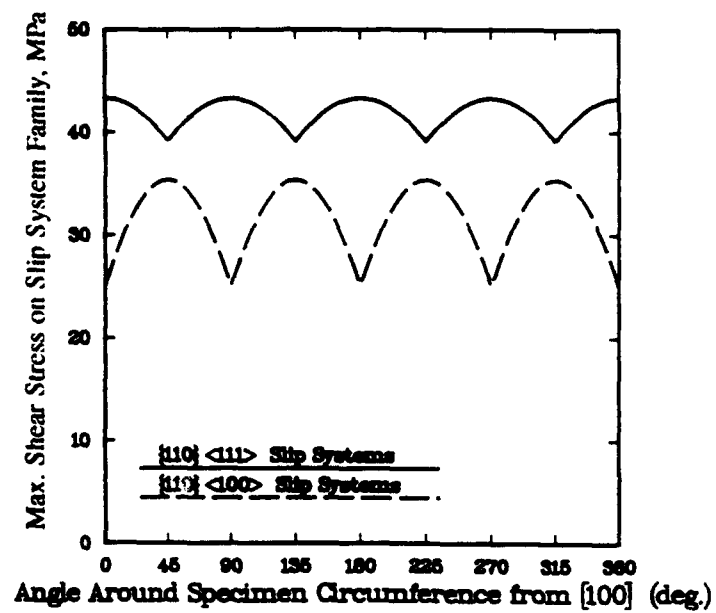


Figure 7. Maximum resolved shear stress on $\langle 111 \rangle \{110\}$ and $\langle 001 \rangle \{110\}$ families of slip systems, $\lambda=0.5$. The troughs indicate a change in the slip system.

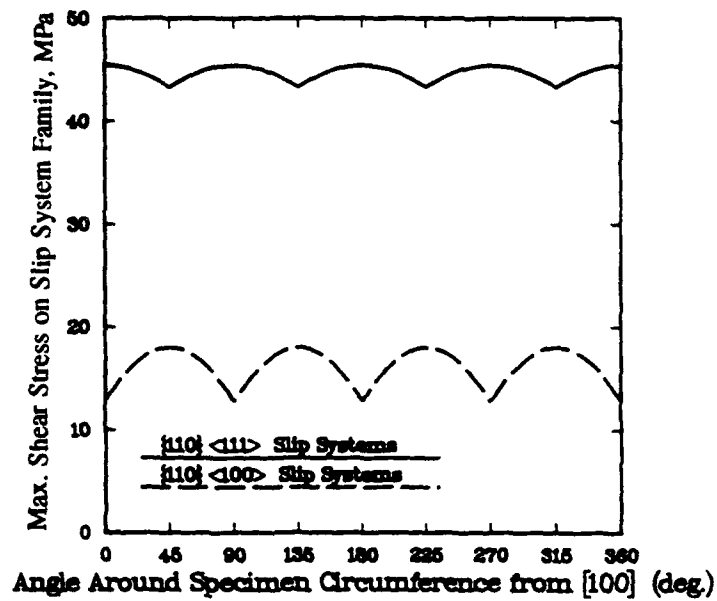


Figure 8. Maximum resolved shear stress on $\langle 111 \rangle \{110\}$ and $\langle 001 \rangle \{110\}$ families of slip systems, $\lambda=0.2$. The troughs indicate a change in the slip system

Table 1. Experimental test matrix for polycrystalline NiAl

Type of Loading	Temperature	Test Conditions	Status
Uniaxial	300 K	Tension	Completed
		Compression	Completed
	900 K	Tension	Completed
Torsion	300 K	Zero Axial Load Hold	Completed
	900 K	Zero Axial Load Hold	In Progress
Multiaxial	300 K	Compression Followed by Torsion	Completed
		Tension Followed by Torsion	In Progress
	900 K	In-phase compression-torsion	In Progress
		In-phase tension-torsion	In Progress